Fuel-Neutral Studies of Particulate Matter Transport Emissions

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Pacific Northwest National Laboratory

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Project ID: ACE056

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PNNL

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Overview

Timeline

- Start - FY09
- Finish - FY17

Budget

- Funding received in FY15 - $200K
- Planned budget for FY16 - $250K

Barriers

- Barriers addressed for enabling of high-efficiency engine technology:
  - B.* Lack of cost-effective emission control
  - C.* Lack of modeling capability for combustion and emission control
  - F.* Lack of actual emissions data on pre-commercial and future combustion engines

* Indexed to list in VTO Multi-Year Program Plan

Partners

- General Motors Company - provide project guidance, support for ERC
- Engine Research Center at University of Wisconsin, Madison - host and operate test engines, perform experiments

Relevance and objectives

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Overall objective: Enable adoption of future high-efficiency engine technologies

Barrier: Lack of actual emissions data on pre-commercial and future combustion engines

Objective: Comprehensive particulate characterization with single-cylinder test engines, guided by industry

2016 Chevy Cruze with 1.4 L turbocharged DI LE2 engine
By Ryan Hildebrand - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=46673960

Barrier: Lack of cost-effective emission control

Objective: Seek to shorten development time of filtration technologies for future engines by improving fundamental understanding of how filter media properties impact back-pressure and filtration efficiency

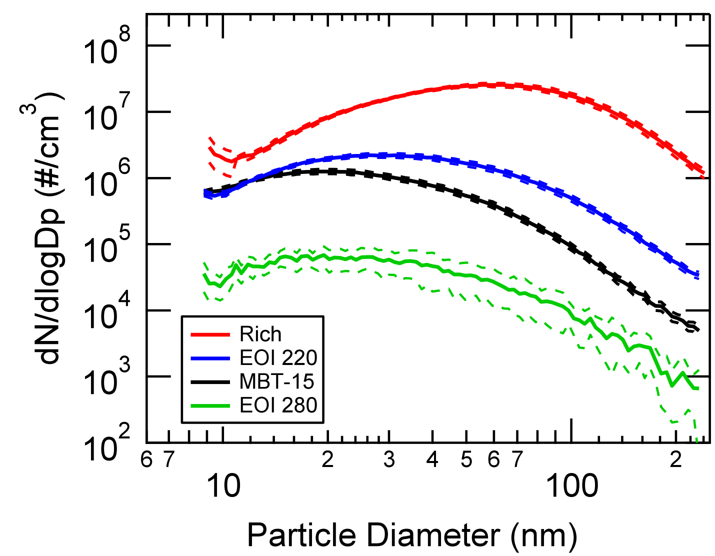
Barrier: Lack of modeling capability for combustion and emission control

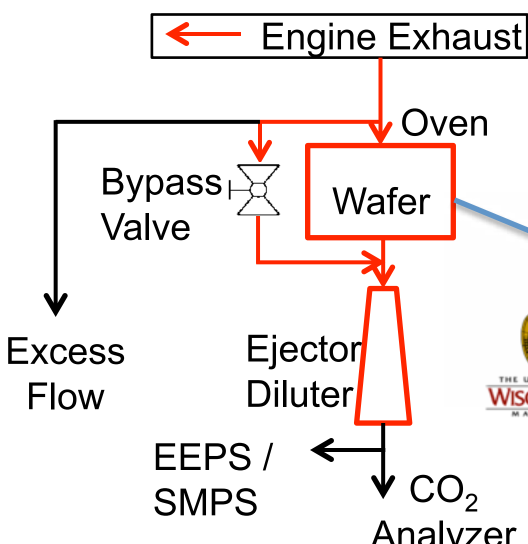
Objective: Develop modeling approaches relevant to the likely key challenge for SIDI filtration – high number efficiency at high exhaust temperatures (implying little soot accumulation in filters)

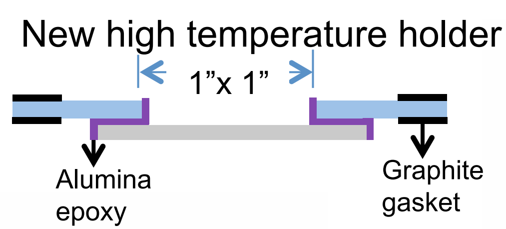
Approach

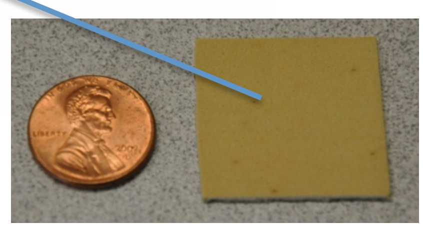
Experiments

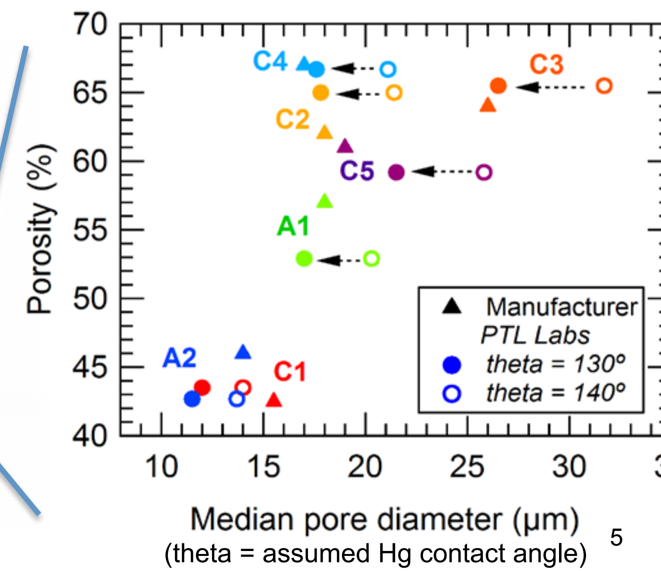
- Three extensive cooperative experimental campaigns have been carried out at the University of Wisconsin Engine Research Center
  - Characterization of exhaust particulates over a wide range of fuels and operating conditions
  - Fundamental studies around soot formation
- EFA filtration experiments
  - Wide variety of filters and particulate populations
  - Current focus is low (but non-zero) soot loadings
  - Refinements in materials and methods (scan rates, etc.)
  - New high-temperature holder simulates close-coupled filter placement





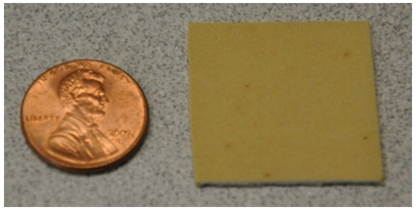


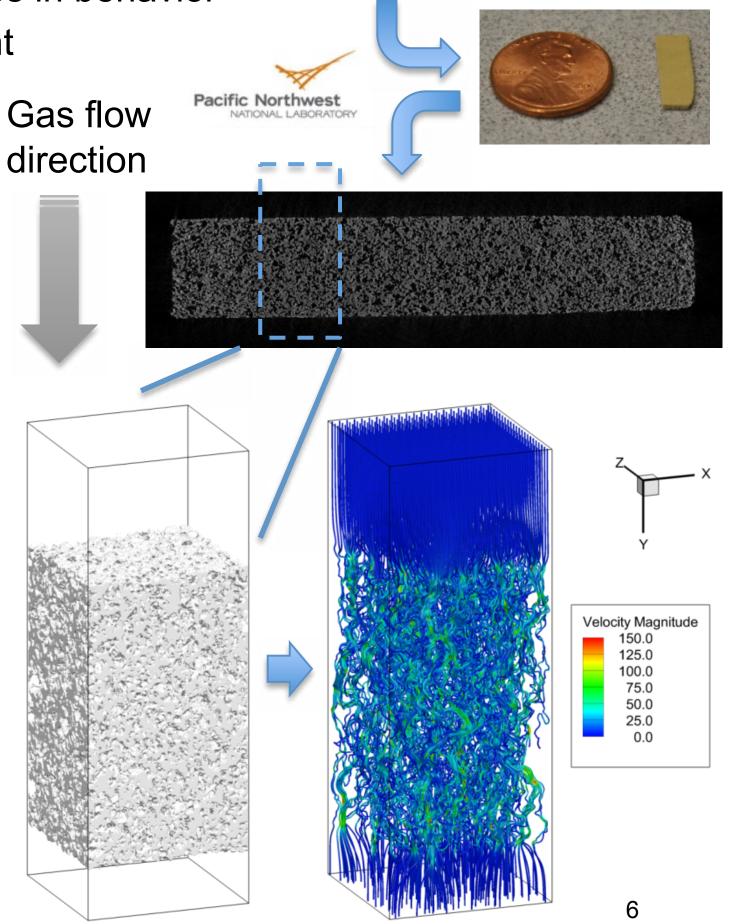


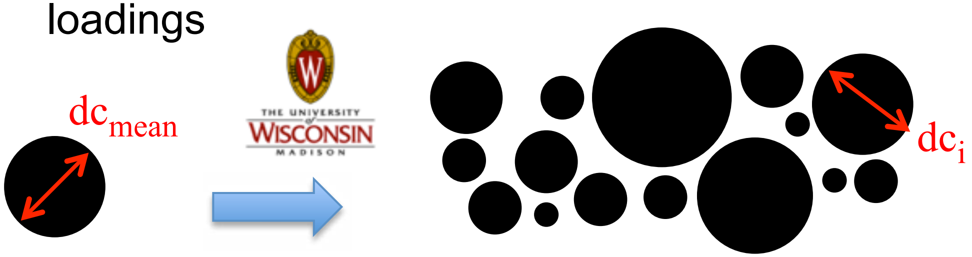


Filter characterization and modeling

- Detailed characterization of filter substrates
  - Hg porosimetry, permeability, exploring other methods
  - Micro X-Ray CT
    - Porosimetry pore sizes do not account for all differences in behavior
    - Differences in texture, microstructure are also important
- Goal is improved device-scale filter models
  - Demonstrated improved clean filter efficiency predictions over baseline unit collector model with modified diffusion capture and U of Wisconsin Heterogeneous Multi-scale Filtration (HMF) model
  - Experiments show that even very small accumulations of soot and ash affect capture efficiency and backpressure
  - Currently seeking general models that require minimum tuning for performance predictions with various substrates, particle size distributions, filter loadings







Particulate characterization

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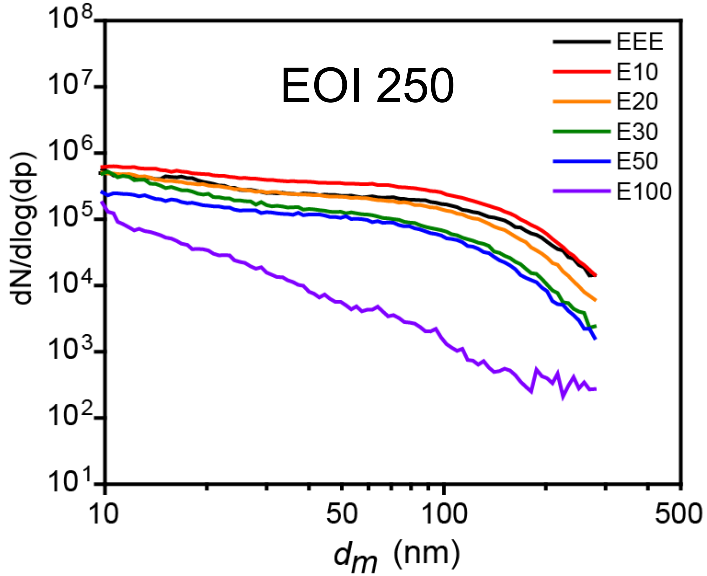
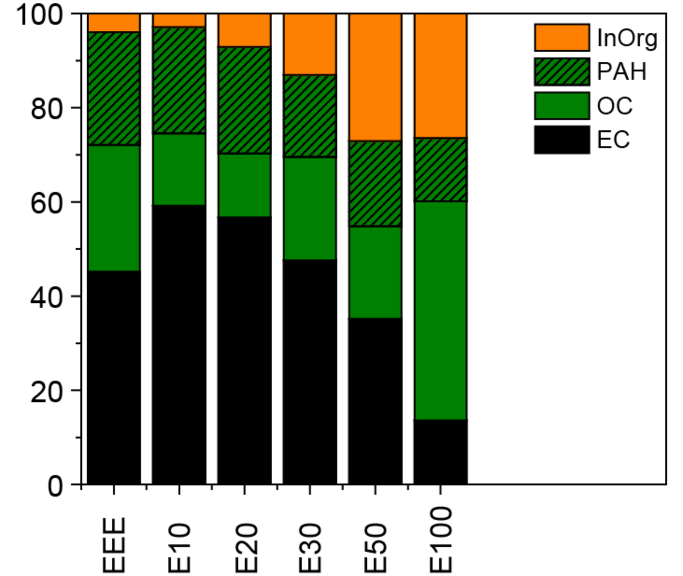
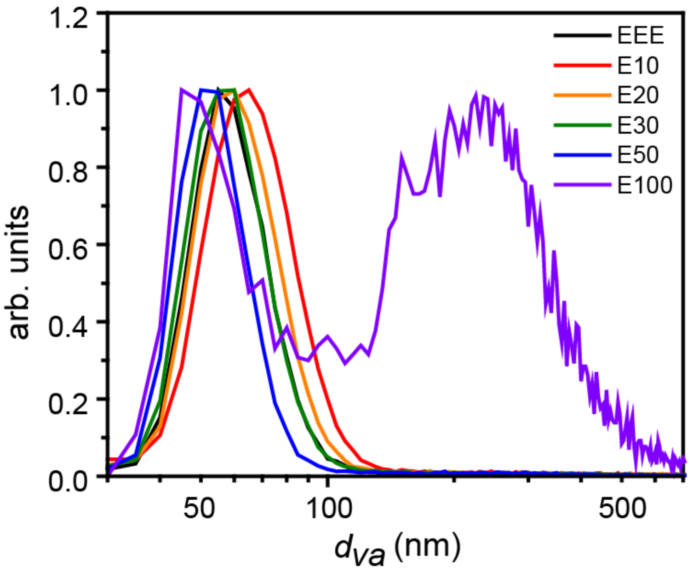
DI PM for different fuel blends: EEE, E10, E20, E30, E50, E100



Average compositions of *fractal* particles

InOrg = inorganics
PAH = polycyclic aromatic hydrocarbons
OC = organic carbon
EC = inorganic carbon

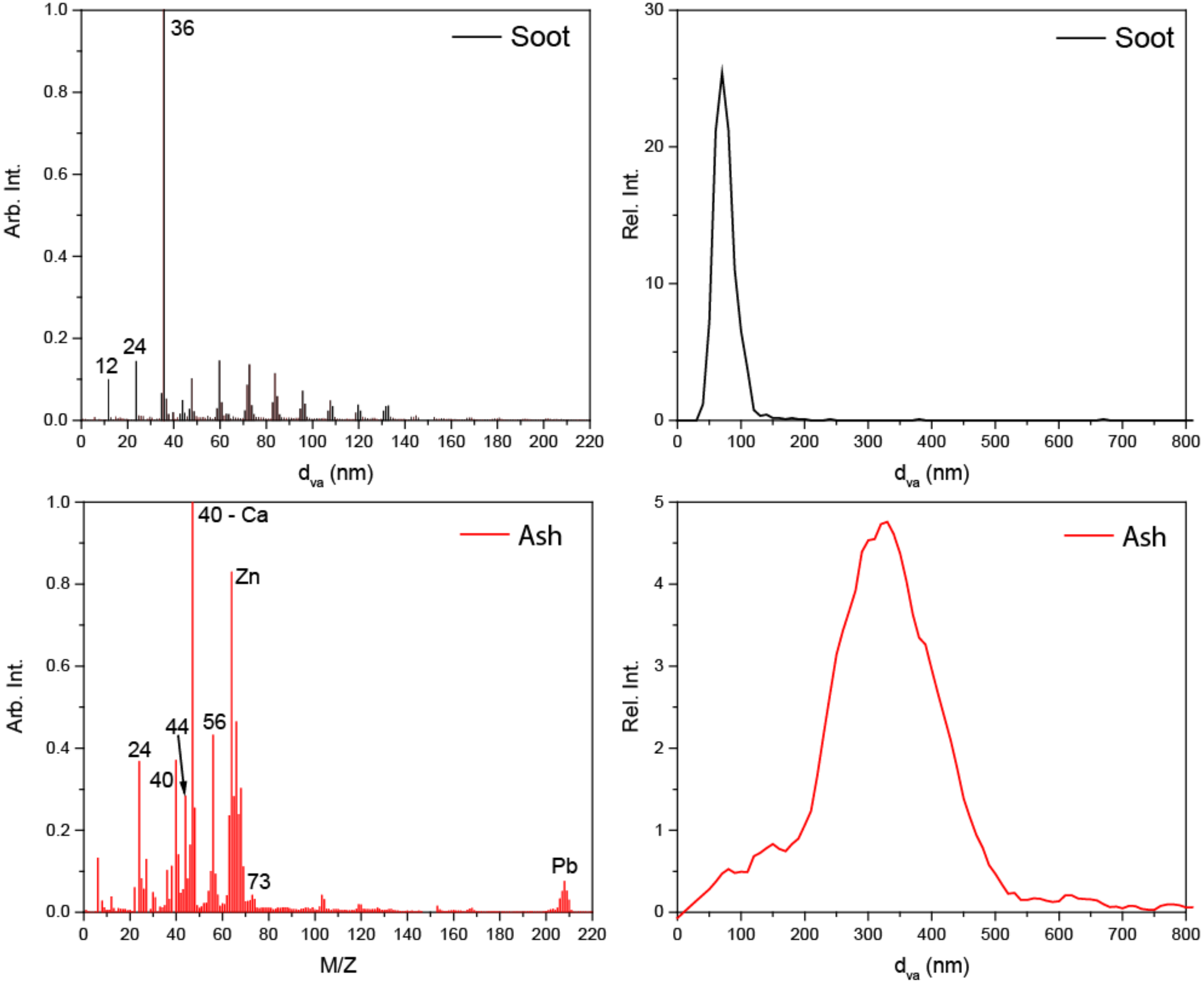




- The vast majority of particles emitted by SIDI engine under all engine operating conditions and fuel blends (except E100) are fractal soot agglomerates
- The average diameter of primary spherules that comprise fractal soot agglomerates varies depending on fuel and engine operating condition
- Fractal soot agglomerates have high organic content, which varies between 40 and 60%, depending on fuel and engine operating condition

Particulate characterization

Composition of *individual* exhaust particles

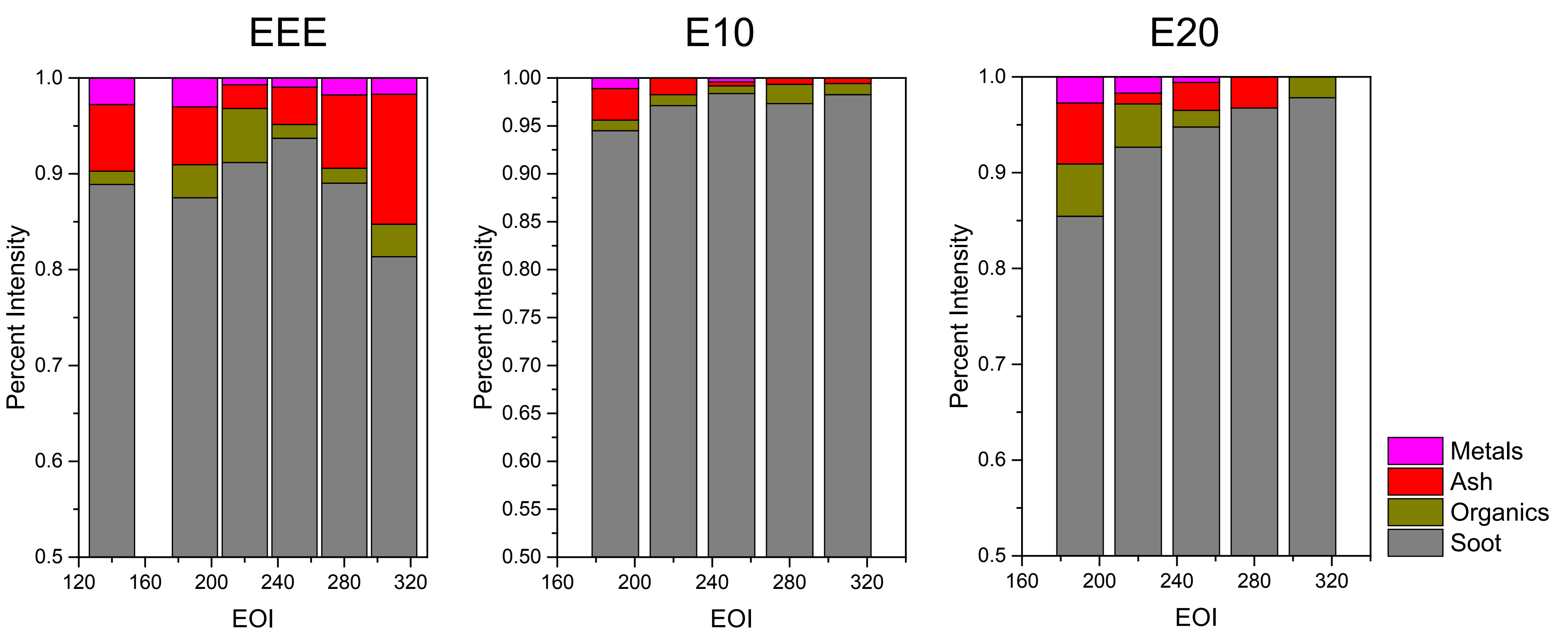


- Exhaust PM represents a complex mixture of particles with various sizes, compositions, morphologies, and shapes
- Examples: fractal soot particles and compact ash particles with larger vacuum aerodynamic diameter (d_{va})

Particulate characterization

Single particle analysis for different fuels: EEE, E10, E20

- Fraction of different particle types depends on engine operating condition and fuel
- Note that the plots below only show range from 0.5 (50%) to 1 (100%), since Soot represent the dominant particle type for these conditions and it is difficult to see the contribution from other particle types

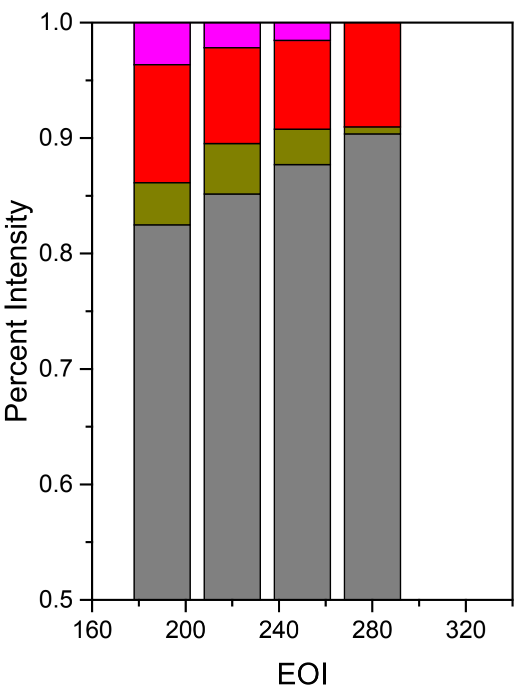


Particulate characterization

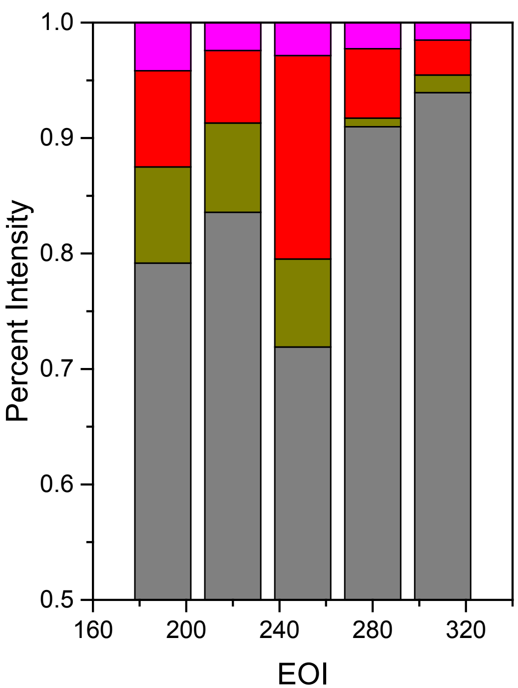
Single particle analysis for different fuels: E30, E50, E100

- Fraction of different particle types depends on engine operating condition and fuel
- Note that the first two plots only show range from 0.5 (50%) to 1 (100%), while the plot for E100 starts at 0
- E100 produces significantly fewer soot particulates. As a result, larger non-fractal particles (ash particles, engine wear & tear) represent significant fraction

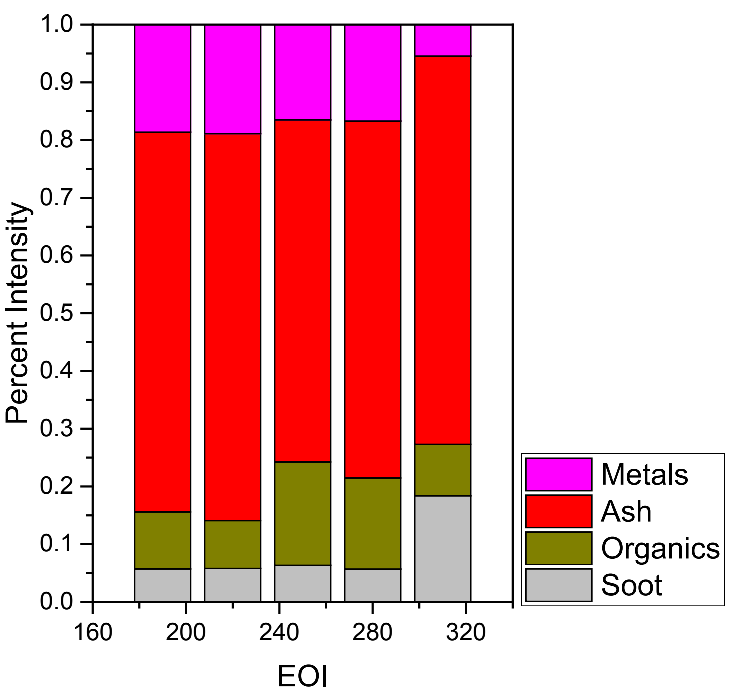
E30



E50



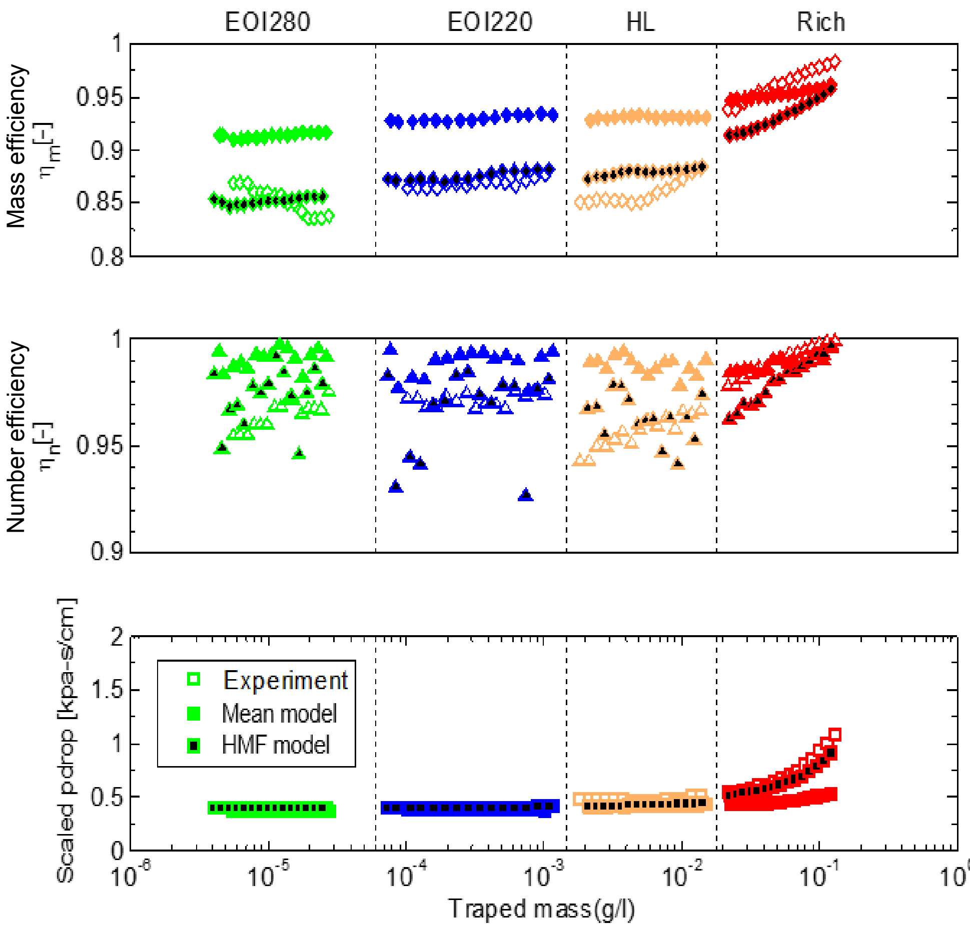
E100



Device-scale modeling

- Standard single unit collector filtration model* and U of Wisc HMF model predictions were compared to new filtration data
- Parameters such as soot deposit porosity in the wall and 'percolation factor' are typically tuned for a specific filter, engine
- Hard to find a model and set of parameters that works well for:
  - Mass efficiency
  - Number efficiency
  - Pressure drop

  under various different engine operating conditions - even for a single filter substrate



Filter sample: C1-60
Face velocity: 2.5 cm/s
Filtration temperature: 125 C

* Konstandopoulos, A. G. and Johnson, J. H., "Wall-Flow Diesel Particulate Filters — Their Pressure Drop and Collection Efficiency," SAE Tech. Pap. 890405, 1989.

Technical accomplishments
New filtration data

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Have obtained a large volume of high quality, repeatable filtration data for a range of substrates, conditions

Example Study: C1 versus A2

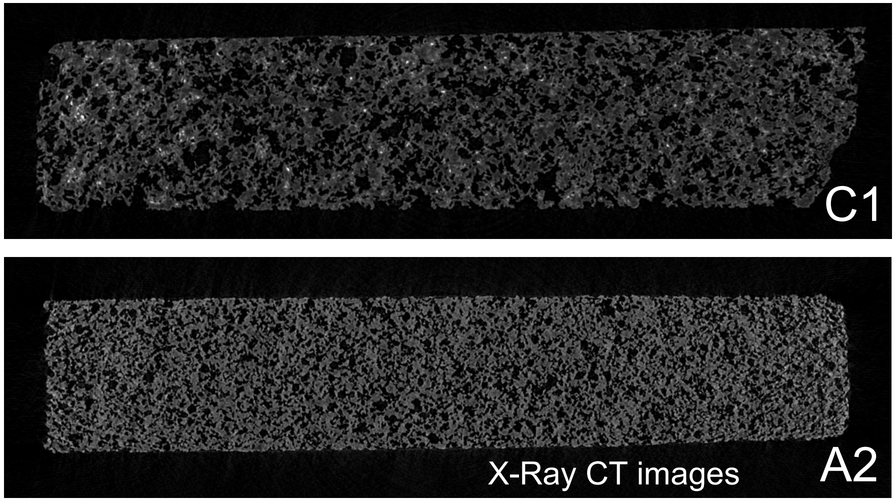
C1 and A2 have similar:

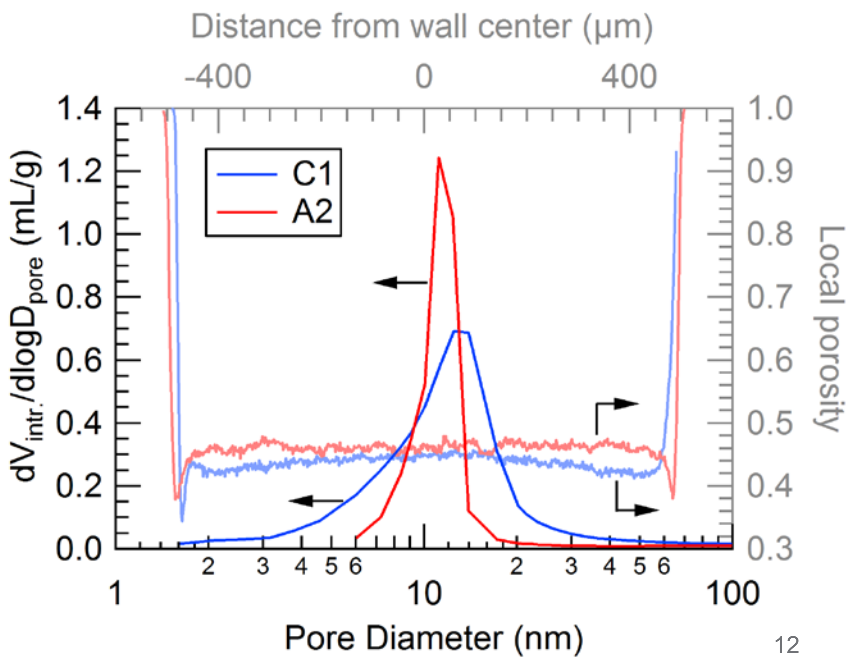
- Pore size
- Total porosity
- Porosity across wall thickness

but differ in:

- Material (Cordierite vs. Aluminum Titanate)
- Width of pore size distribution (W)
- Clean permeability (~12% difference)

Batch	Por. (%)	MPD (μm)	$\sigma_{\mu m}$	***W***	Th. (mm)	Perm. $*10^{-13}$ (m^2)
C1	43	12	4.3	0.55	1.05	6.8±0.1
A2	43	11.4	0.8	0.24	1.05	7.6±0.1





New filtration data

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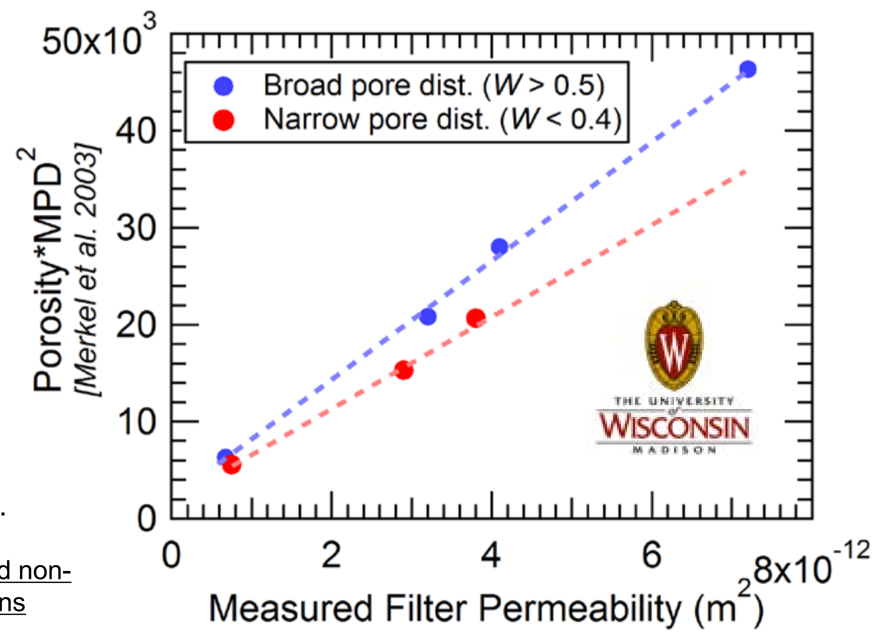
Batch	MPD (µm)	$\sigma_{\text{log-norm}}$	*W*
C1	12	0.31	0.55
C2	17.9	0.19	0.55
C3	26.6	0.20	0.52
C4	17.6	0.13	0.36
C5	21.75	0.18	0.49
A1	17	0.15	0.39
A2	11.4	0.1	0.24

MPD = median pore diameter

$$W = \frac{d_{50} - d_{10}}{d_{50}}$$

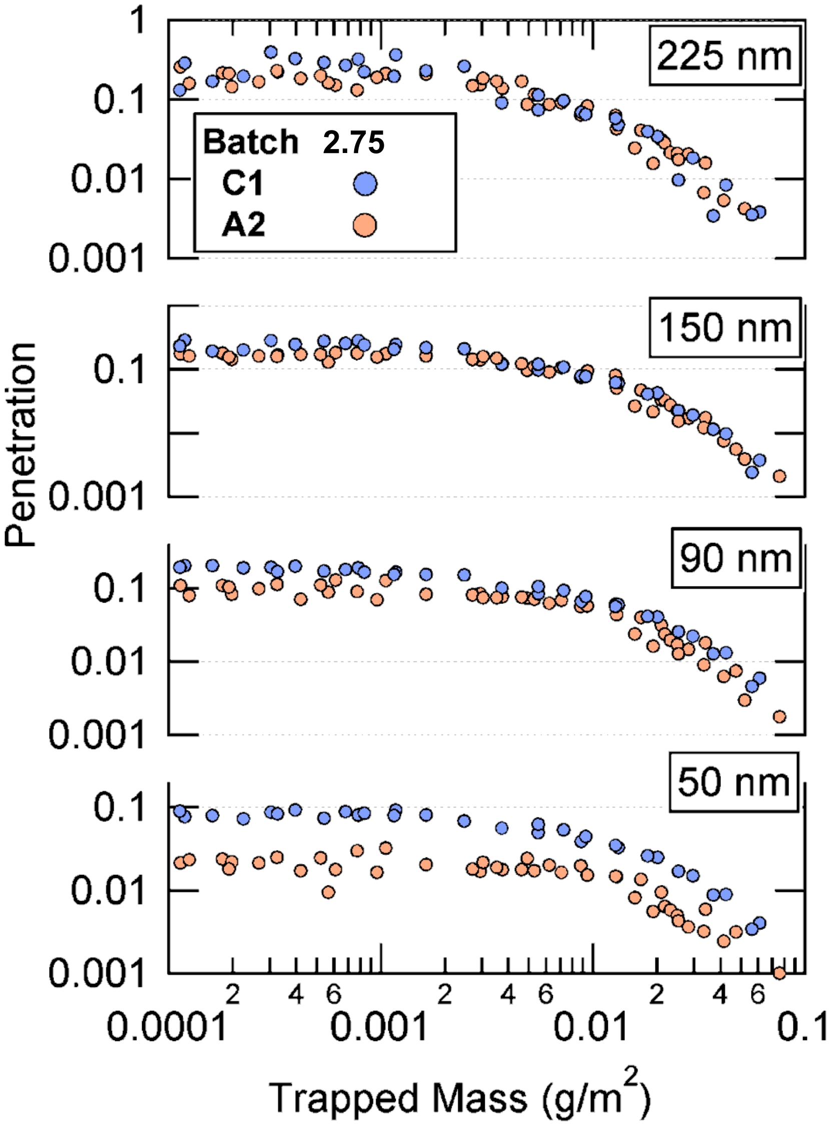
Clean permeability ∝ Porosity · MPD^2

- Merkel et al.* proposed the "W" metric for width of pore size distribution and related it to loaded backpressure
- Size distribution width metrics are shown here for eight of the substrates included in this study
- Clean permeability seems to depend on W as well as porosity and pore size
- Lower W has been associated with better pore connectivity



* Merkel, G. A., W. A. Cutler, T. Tao, A. Chiffey, P. Phillips, M. V. Twigg and A. Walker (2003). New cordierite diesel particulate filters for catalyzed and non-catalyzed applications. 9th Diesel Engine Emissions Reduction Conference, Newport, Rhode Island.

New filtration data



- Penetration of large particles similar
  - Likely dominated by interception
- Significant difference in penetration of small particles
  - Likely dominated by diffusion
  - Better pore connectivity in A2 could contribute to higher efficiency through:
    - Lower interstitial velocities
    - More uniform access of flowing gas to internal surface area

Filter substrates: C1, A2
Face velocity: 2.75 cm/s
Filtration temperature: 125 C

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Technical accomplishments

New filtration data

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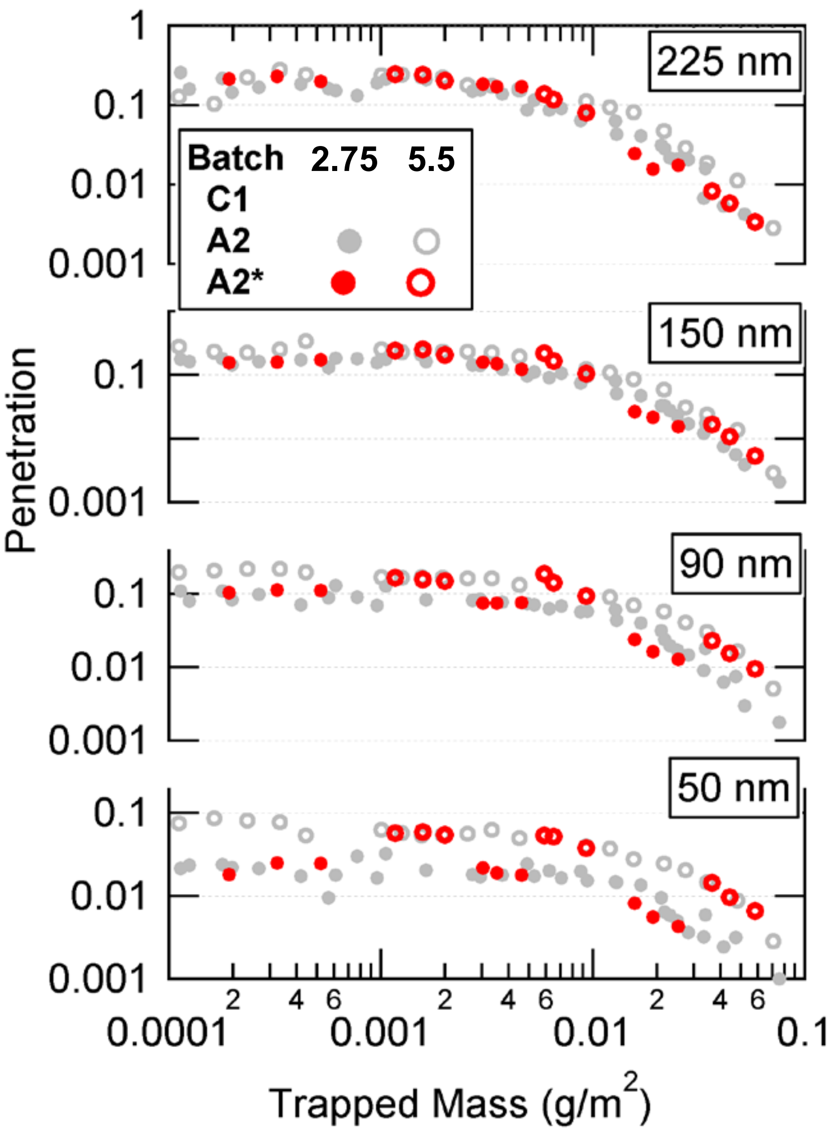

- Checked impact of sample to sample variability - trends still consistent across multiple samples
- Changing velocity had little impact on removal of large particles
  - Consistent with theory - interception term has no velocity dependence
- Changing velocity had significant impact on removal of small particles
  - Trend again consistent with theory

Filter substrate: A2
Face velocities: 2.75, 5.5 cm/s
Filtration temperature: 125 C

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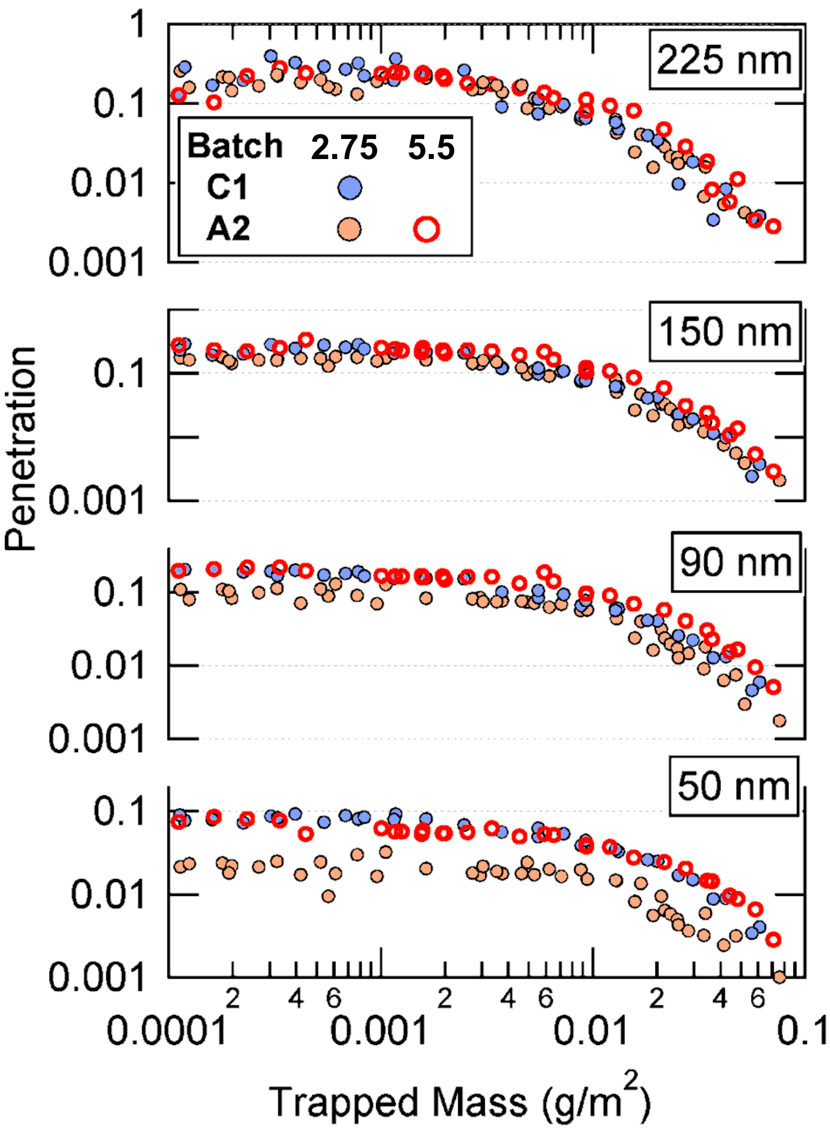
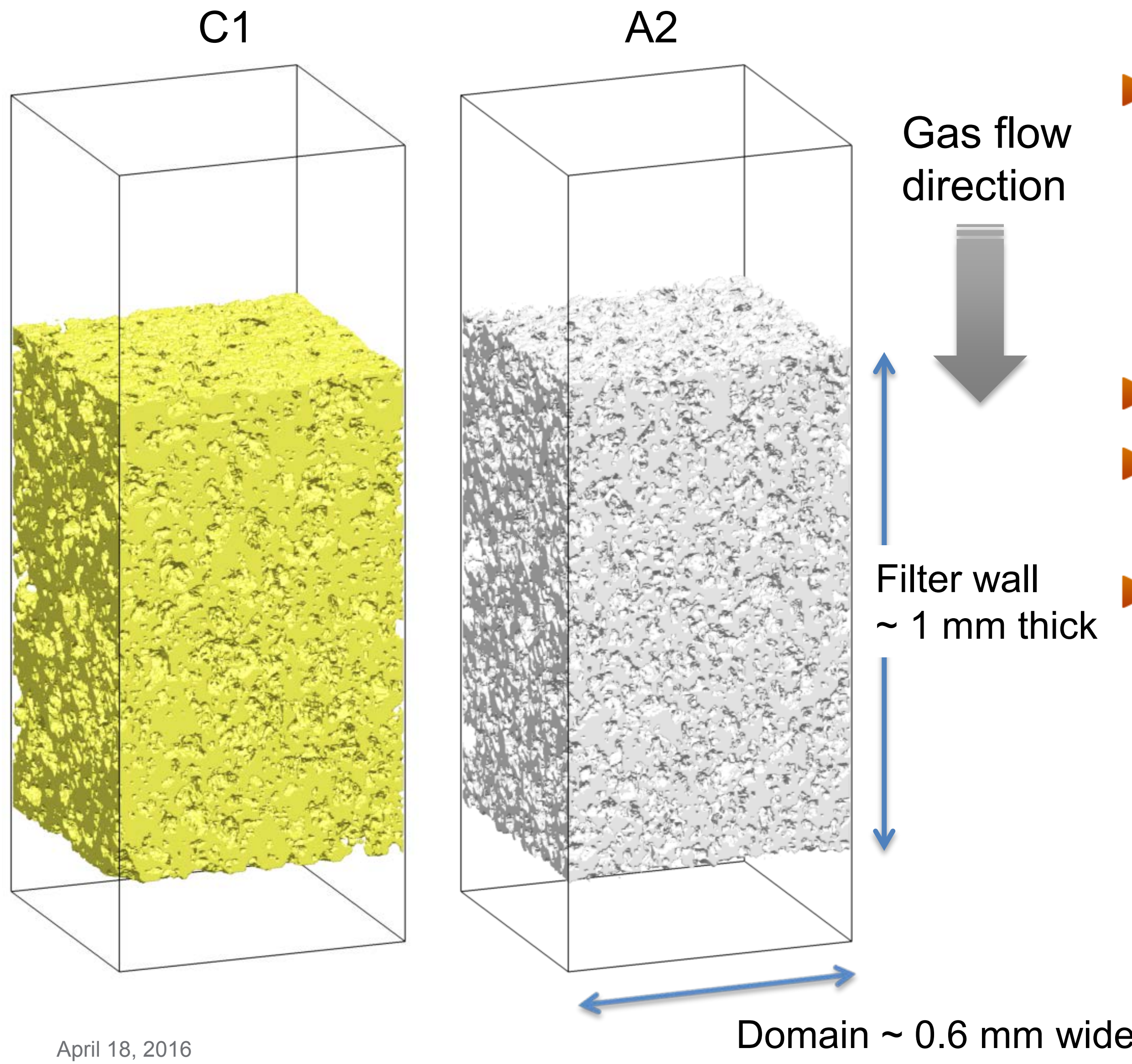
New filtration data



- A2 performance for removal of small particles equals that of C1 at half the filtration velocity
- Since back-pressures are comparable, A2 would seem to have a clear advantage
- Consistent with longstanding consensus that narrow particle size distribution is better
- Little difference in performance for large particles

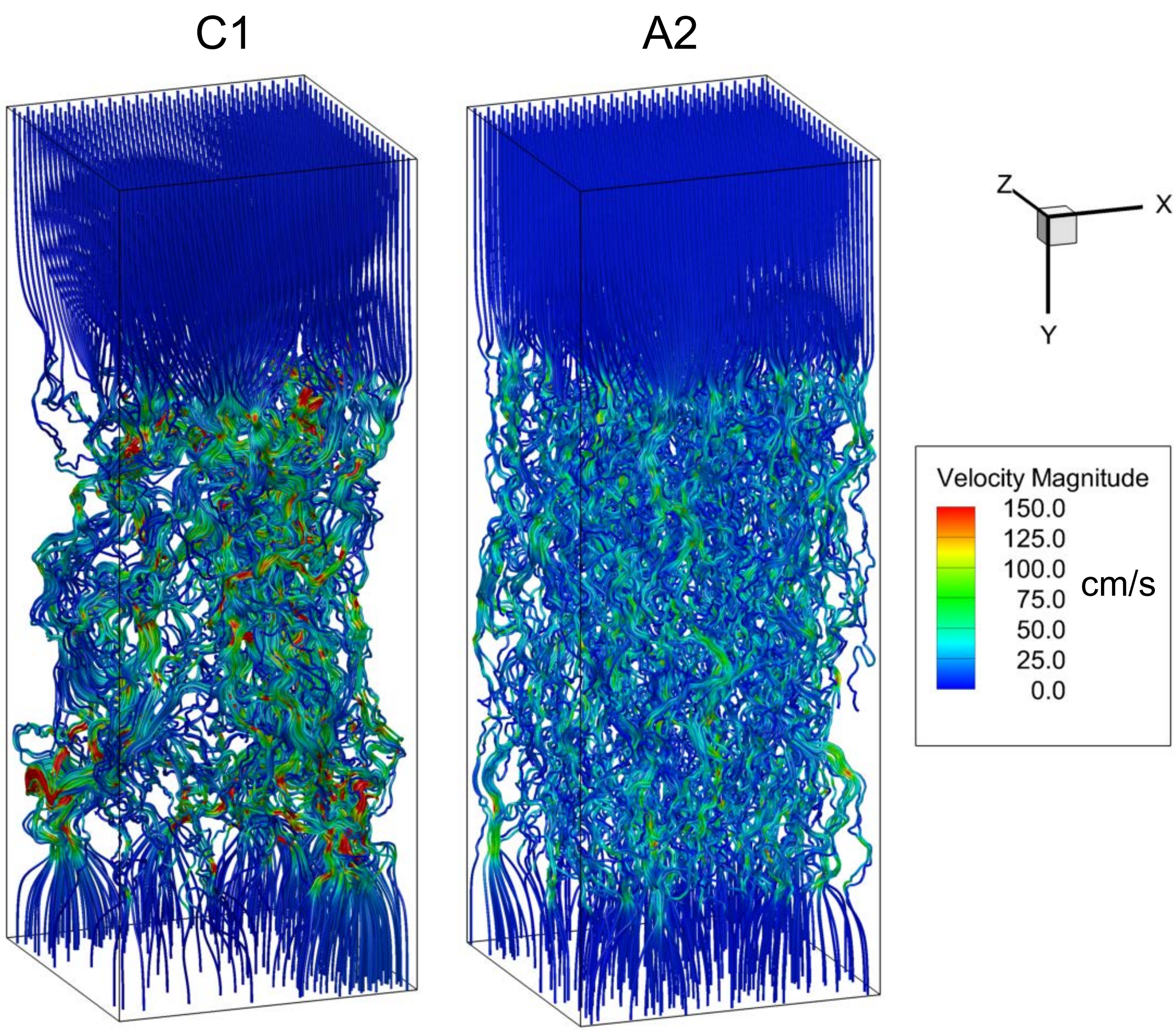
Filter substrates: C1, A2
Face velocities: 2.75, 5.5 cm/s
Filtration temperature: 125 C

Lattice Boltzmann simulations



- LB flow simulations carried out on small sections of 3D reconstructions from X-Ray CT data
- Resolution: 3.3μm
- Approach velocity: 3.64 cm/s
- ~15 million computational cells per simulation

Lattice Boltzmann simulations



- Streamlines colored according to local velocity
- Fewer major flow paths per volume through C1
- Higher local velocity in bottlenecks
- Better flow distribution in A2 gives the exhaust access to more surface area for capture by diffusion
- Lower velocities also mean longer residence times in the wall

Lattice Boltzmann simulations

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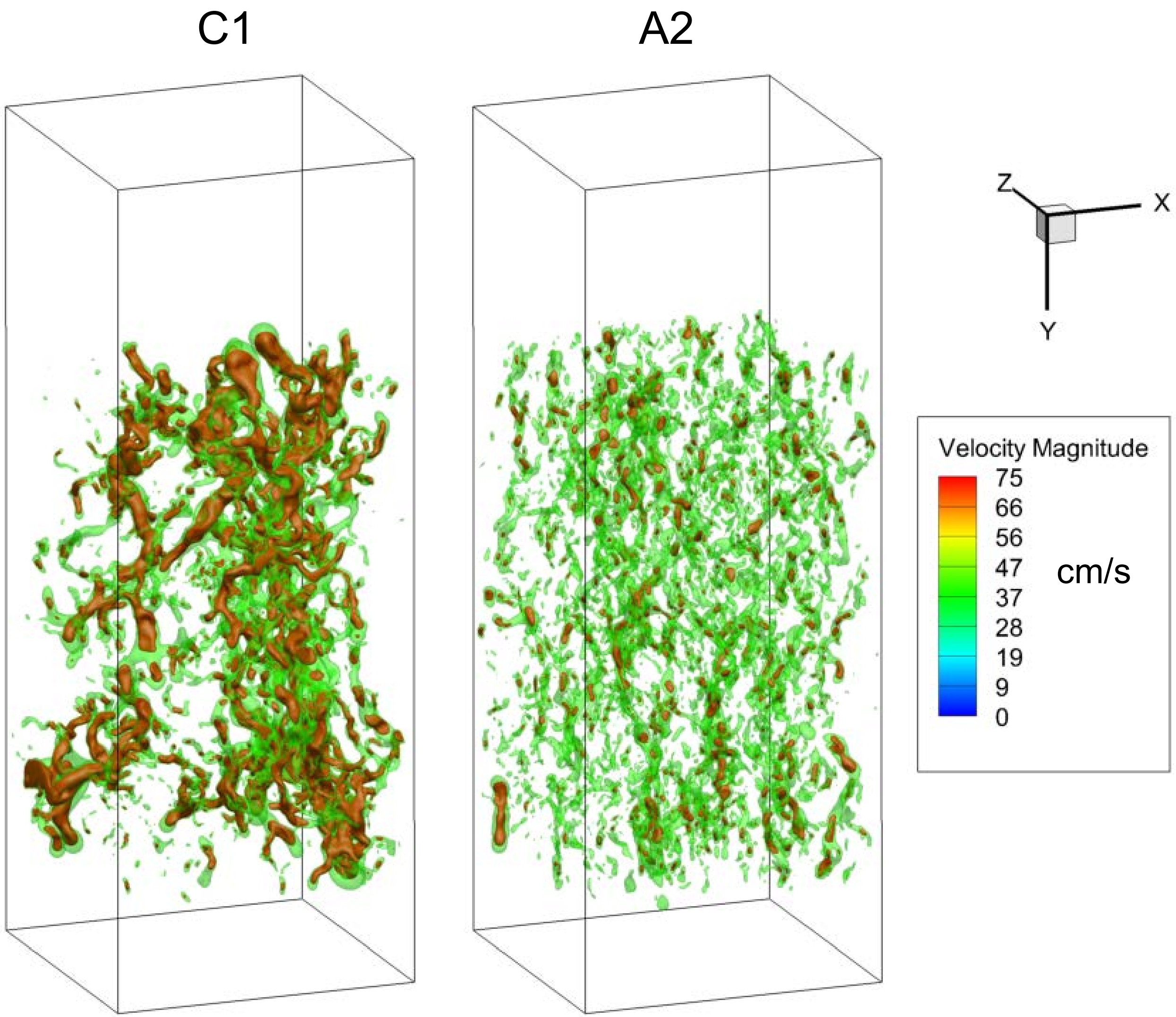
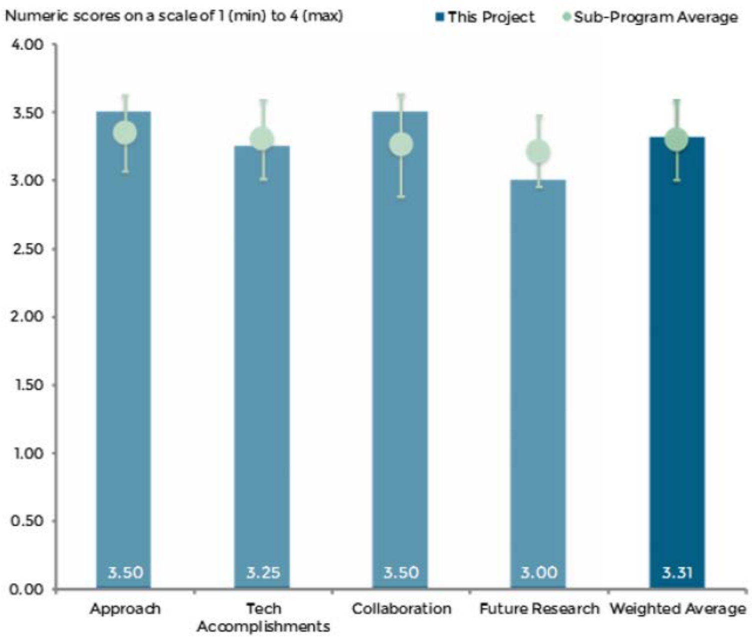


- Velocity iso-surfaces at 75, 40 cm/s
- Smaller high-velocity regions are more distributed throughout the wall volume in A2
- At these thresholds, some of the largest, twisting paths through portions of the C1 filter wall are visible

FY15 reviewer comments



- Excellent collaboration, good communication
- "These fundamental studies on gasoline particulate drivers are important to guide future direction."
- "…technical accomplishments in this area have been impressive."
- "…this project takes a comprehensive approach in characterizing the particulate matters for gasoline direct injection (GDI) engines using various fuels and at various engine operating conditions."
- "Well coupled to ACEC combustion strategies and future GDI engines"
- "Extensive work on fuel effects on in-cylinder PM formation, PM and filter characterization, and PM filtration behavior."

- "…not clear to what level the experimental results have improved the feasibility or provided direction of change in the proposed model." "Development/refinement of filter models based on test data should be pushed harder with higher priority."

  Agreed. Refinement of filter models will be our top priority moving forward.

- "Given the potential future application of multi-functional filter devices such as GPF and SCRF, the effects of catalyst washcoat on filtration efficiency, pressure drop, and gaseous emissions conversions need to be investigated in more detail."

  Catalyzed filter samples have been procured and added to the project for filtration experiments and micro-scale characterization in FY16.

- "Need to include the effects of ash on backpressure and reactivity of the soot."

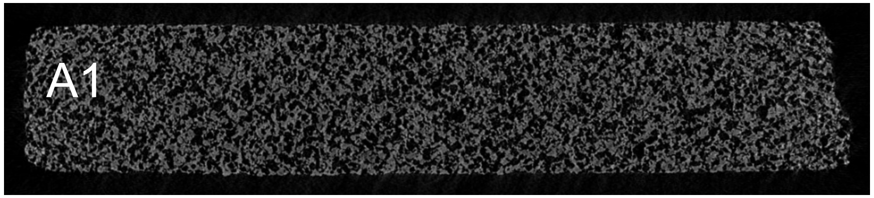
  Effects of ash on backpressure and filtration efficiency have been investigated over the past year in low temperature experiments. Ash will also be considered in high-temperature experiments which are commencing now.

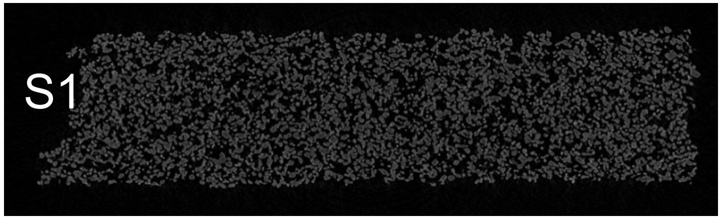
Collaborations

- Major Partners
  - General Motors Company (Industry): Provide funding (supporting full-time doctoral student working on improved models), hardware, expertise, and operational guidance for engine experiments at the ERC. Advise on project direction and priorities.
  - Engine Research Center at University of Wisconsin, Madison (Academic): Operate test engine - including shakedown tests, independent experiments, and cooperative experiments. Assist in analysis and publication of data. Develop improved device-scale modeling techniques.
- Analysis subcontracts
  - Micromeritics
  - Particle Tech Labs
  - Micro Photonics
- Filter suppliers
  - Corning Incorporated
  - Ibidin
  - NGK
  - Sumitomo

Remaining challenges and barriers

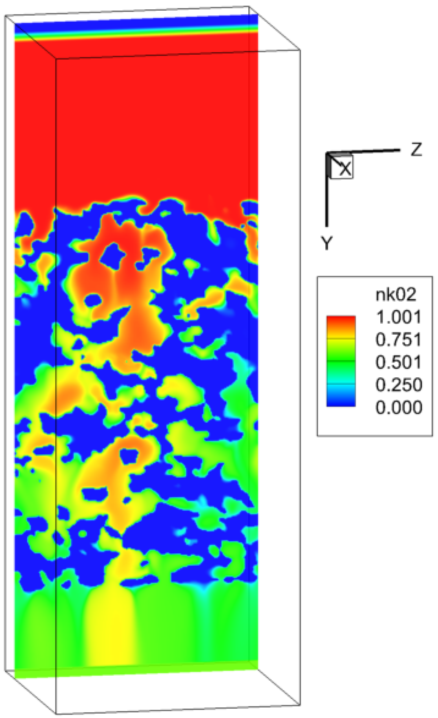
- Readily available characterization tools such as mercury porosimetry seem inadequate to completely describe the structural features of filters that determine performance
- The rich datasets available from 3-D imaging show clear differences between materials and products, but a set of quantitative, descriptive parameters that correlates directly to performance remains elusive
- More general models are needed, which will allow prediction of filter performance as a function of well-defined structural properties over a wide range of engine operating conditions
- Need filtration data for continuous regeneration conditions with little soot in the filter, representing close-coupled GPF

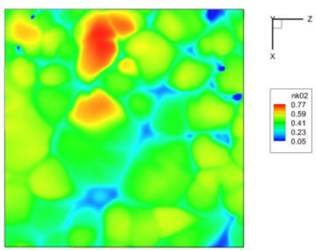




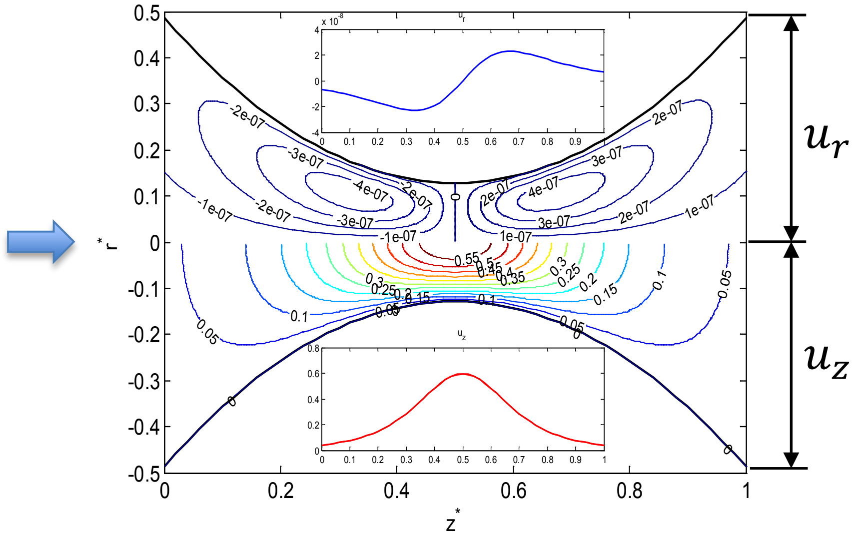
Future work

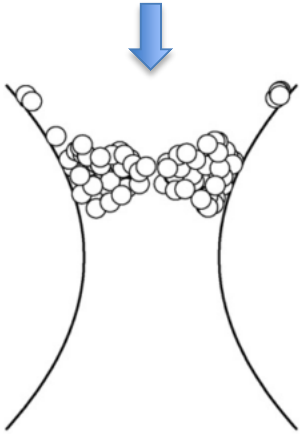
- Further expand set of tested filter samples, including catalyzed filter substrates
  - EFA tests
  - Micro X-Ray CT, analysis
- Test 3rd generation high-temperature sample holder/gasket system
- Perform filtration experiments representative of close-coupled filter placement
- Evaluate new porous media characterization techniques
  - Extrusion flow porometry
  - Extrusion porosimetry
- Complement experimental characterization methods with analysis of 3D micro X-Ray CT data and pore-scale simulations for various substrates tested
- Evaluate constricted tube filter model, comparing to experimental data
- Develop improved filtration models

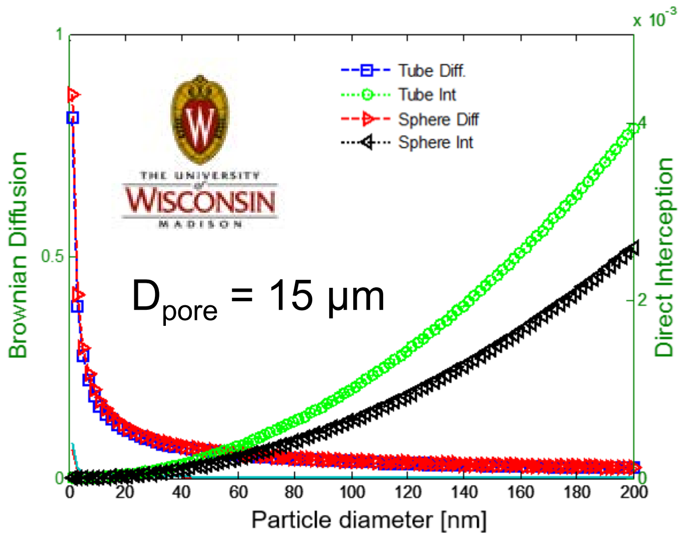




Evaluation of alternative filter models



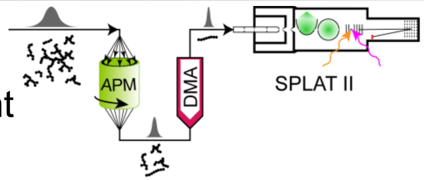




- Goal is filter model that gives better predictions with minimal tuning to match data
- In addition to spherical unit collector models, other alternatives are being explored
- One candidate is the constricted tube model*

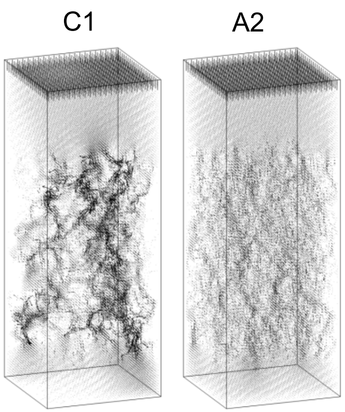
* Tien, C. and Payatakes, A., "Advances in deep bed filtration," AIChE J., no. 5, pp. 737–759, 1979.

Summary/Conclusions



- Completing analysis of SIDI particulate characterization data
  - Various particle types present in exhaust in different proportions under different engine operating conditions
- EFA filter testing capability further developed/refined
  - Developed methods for real-time filter loading estimates from particle populations
  - Evaluated effects of particle sizer scan rates on data
  - Improved low temp materials/methods to avoid particle formation
  - Developed 3rd generation high-temperature sample holder/gasket system

- Began building a large set of high quality fundamental filtration data
  - Evaluated sample-to-sample variation
  - Confirmed repeatability
  - Collected data for multiple substrates covering a wide range of filter properties
  - Quantified effects of low soot and ash loadings on performance
- Development of filter characterization approaches
  - Evaluating other analytical methods, including extrusion porometry and flow porosimetry
  - X-Ray CT data and micro-scale flow simulations are useful in explaining differences in substrate performance
- Exploring alternatives to standard unit collector filtration model



Technical Back-Up Slides

Schedule for FY 14 cooperative experiments

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	Monday 6/9/2014	Tuesday 6/10/2014	Wednesday 6/11/2014	New Thursday 6/12/2014	New Friday Plan 6/13/2014	Saturday 6/14/2014	Sunday 6/15/2014	Monday 6/16/2014	Tuesday 6/17/2014	Wednesday 6/18/2014	Thursday 6/19/2014	Friday 6/20/2014
Fuel:	**EEE**	**EEE**	**EEE**	**EEE**	**EEE/TRF**	**E10/E20/E30**	**E10/E20**	**E50/TRF/Iso**	**EEE/E30**	**E50/E100 ISOOCTANE**	**EEE**	**EEE**
DI / PMPV:	**DI**	**DI**	**DI**	**PMPV**	**DI**	**PMPV**	**DI**	**PMPV**	**DI**	**DI**	**DI**	**DI**
8:00	Setup & Troubleshoot	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup	Warmup
9:00		Trial Run	EFA Troubleshoot	SOC NFB Phi = 0.98	EOI 220 Phi = 0.98	SOC NFB E10 Phi = 0.98	EOI 220 E10 Phi = 0.98	SOC NFB E50 Phi = 0.98	Sandeep Tests	EOI 220 E50 Phi = 0.98	Heavy Load Characterization	Probing C1, Heavy Load, Filtration
10:00				SOC - Low DR Phi = 1.50	EOI 340 Phi = 0.98	SOC E10 Phi = 1.43	EOI 190 E10 Phi = 0.98	SOC E50 Phi = 1.63	EOI 220 EEE Phi = 0.98	EOI 280 E50 Phi = 0.98		Probing
11:00		EOI 220 Characterization		High Load Phi = 1.50	EOI 250 (min part) Phi = 0.98	SOC E10 Phi = 1.50	EOI 250 E10 Phi = 0.98	SOC E50 Phi = 1.56	EOI 310 EEE Phi = 0.98	EOI 250 E50 Phi = 0.98		Filtration
12:00		Rich Characterization		Low Speed Phi = 1.50	EOI 140 Phi = 0.98	Change Fuel	EOI 280 E10 Phi = 0.98	Change Fuel SOC NFB TRF Phi = 0.98	EOI 190 EEE Phi = 0.98	EOI 190 E50 Phi = 0.98		Probing Filtration
13:00				SOC - Low DR Phi = 0.98	EOI 220 - Random Fire Phi = 0.98	SOC NFB E20 Phi = 0.98	EOI 310 E10 Phi = 0.98	SOC TRF Phi = 1.50	EOI 280 EEE Phi = 0.98	EOI 310 E50 Phi = 0.98	Probing through Bypass and Clean Filter	Probing
14:00		EOI 280 Characterization	EOI 220 Characterization	High Load Phi = 1.40	Change Fuel EOI 220 TRF Phi = 0.98	SOC E20 Phi = 1.46	Change Fuel EOI 220 E20 Phi = 0.98	SOC TRF Phi = 1.40	EOI 250 EEE Phi = 0.98	Change Fuel EOI 220 E100 Phi = 0.98		Packing
15:00		MBT -15 Characterization	C1, EOI 220, Filtration (Wash 15)	SOC Phi = 1.40	EOI 340 TRF Phi = 0.98	SOC E20 Phi = 1.52	EOI 250 E20 Phi = 0.98	SOC TRF Phi = 1.35	Change Fuel EOI 220 E30 Phi = 0.98	EOI 190 E100 Phi = 0.98		
16:00				Low Speed Phi = 1.40	EOI 250 (min part) TRF Phi = 0.98	Change Fuel	EOI 280 E20 Phi = 0.98	Change Fuel	EOI 310 E30 Phi = 0.98	EOI 250 E100 Phi = 0.98		
17:00		EFA Troubleshoot	EFA Troubleshoot	SOC SPIKE Phi = 1.35	EOI 140 TRF Phi = 0.98	SOC NFB E30 Phi = 0.98	EOI 190 E20 Phi = 0.98	SOC NFB ISO Phi = 0.98	EOI 190 E30 Phi = 0.98	EOI 280 E100 Phi = 0.98	C2, Heavy Load, Filtration	
18:00				SOC Normal Phi = 1.35		SOC E30 Phi = 1.50	EOI 310 E20 Phi = 0.98	SOC ISO Phi = 1.50	EOI 280 E30 Phi = 0.98	EOI 310 E100 Phi = 0.98	Probing Filtration	
19:00			Heavy Load Characterization			SOC E30 Phi = 1.55	EOI 220 E20 Phi = 0.98		EOI 250 E30 Phi = 0.98	EOI 220 E100 Phi = 0.98	Probing	
20:00			C2, Cold probing						EOI 220 E30 Phi = 0.98			
21:00												
22:00												

Approach

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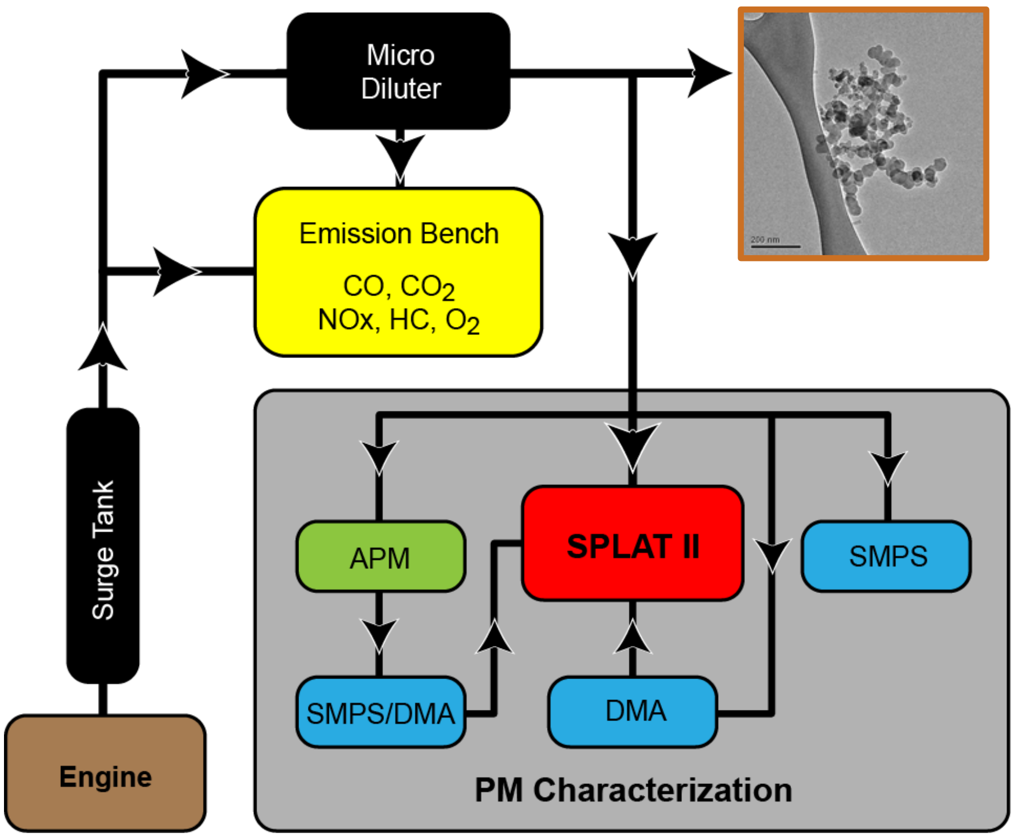
- Advanced test engines at the UW ERC allow experiments with candidate next-generation gasoline engine technologies
- Highly detailed PM characterization is enabled by an array of advanced instruments and methods
- Exhaust PM represents a complex mixture of particles with various sizes, shapes, morphologies, and compositions that can be identified and characterized as a function of engine operating condition and fuel



- **SMPS:**
  - ✓ size distributions (mobility), d_m
- **SPLAT II:**
  - ✓ single particle size (aerodynamic), d_{va}
  - ✓ single particle composition, *MS*
- **DMA/SPLAT:**
  - ✓ effective density, ρ_{eff}
  - ✓ fractal dimension, D_{fa}
  - ✓ primary spherule diameter, d_p
- **APM/DMA/SPLAT:**
  - ✓ particle mass, m_p
  - ✓ mass vs. mobility diameter relationship
  - ✓ fractal dimensions, D_{fm}, D_{pr}
  - ✓ primary spherule diameter, d_p
  - ✓ number of spherules, N_p
  - ✓ void fraction, Φ
  - ✓ dynamic shape factors (χ_t, χ_v)
  - ✓ real-time shape-based separation

Exhaust Filtration Analysis (EFA) experiments

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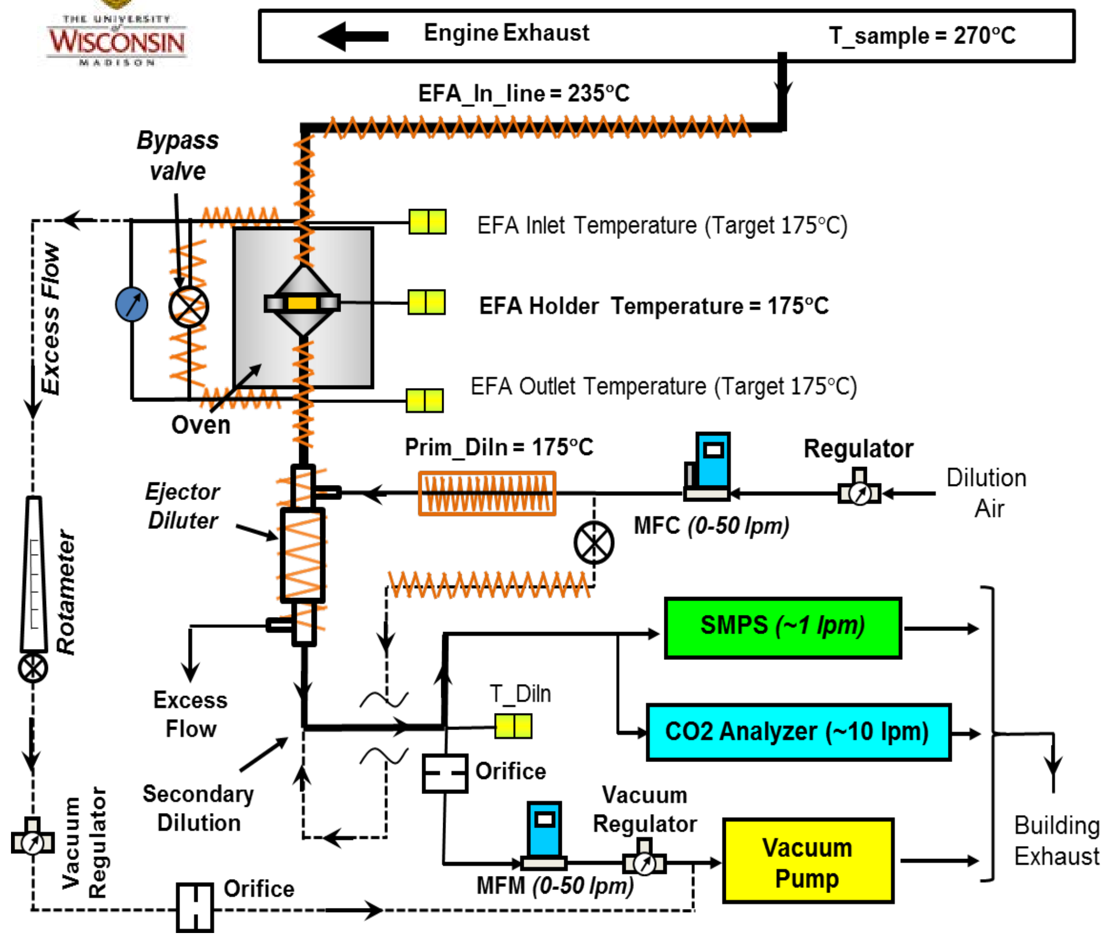

- Filtration experiments conducted with flat wafer samples and exhaust from single cylinder test engine
- Particulates measured with Scanning Mobility Particle Sizer (SMPS) and Engine Exhaust Particle Sizer (EEPS)

See SAE-2014-01-1558

EFA Modifications
High temperature setup

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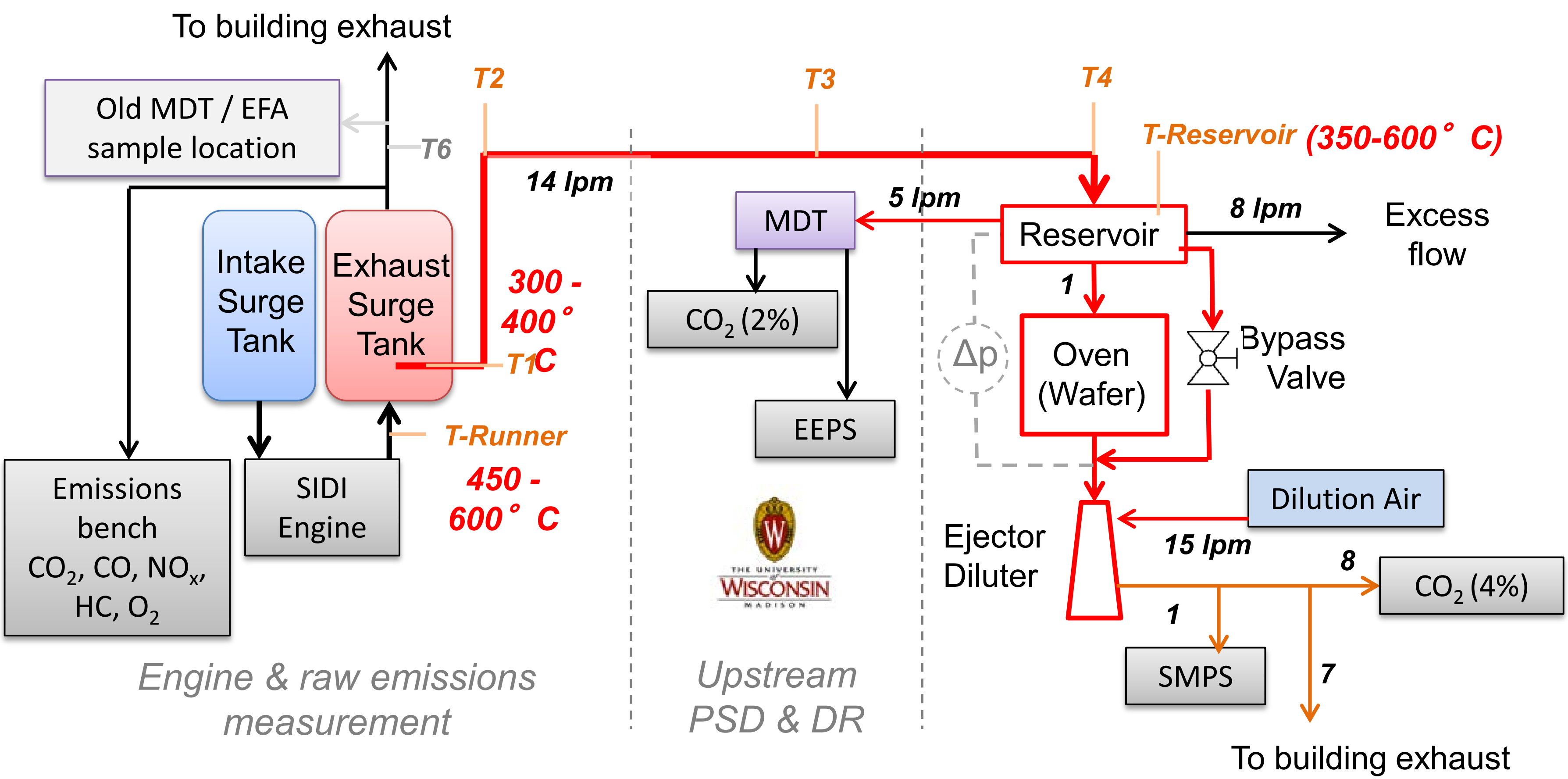

- *Impact of modified setup & sampling location on PSD was relatively small*

Heterogeneous Multi-scale Filtration (HMF) model

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- Mean collector size (standard approach)
  - Mean pore size and mean porosity

$$\eta_{mean}(dp_i)=1-\exp\left(-\frac{3*\eta_{comb}(dp_i,dc_{mean})*(1-\epsilon_{mean})*w}{2*\epsilon_{mean}*dc_{mean}}\right)$$

- HMF
  - Use a cluster of collectors with different diameters to represent the complex porous structure
  - Pore size PDF and porosity distribution

$$\eta_i(dp_i,dc_i)=1-\exp\left(-\frac{3*\eta_{comb}(dp_i,dc_i)*(1-\epsilon_j)*w}{2*\epsilon_j*dc_i}\right)$$

$$\boxed{\eta_{HMF}(dp_i)=\frac{\int \eta_i(dp_i,dc_i)\cdot dc_i^2\cdot pdf(dc_i)\,d(dc_i)}{\int pdf(dc_i)\cdot dc_i^2\,d(dc_i)}}$$